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Tunneling and Energy Splitting in Ising Models

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Abstract

The energy splitting E_{0a} in two and four dimensional Ising models is measured in a cylindrical geometry on finite lattices. By comparing to exact results in the two dimensional Ising model we demonstrate that E_{0a} can be extracted very reliably from Monte Carlo calculations in practice. In four dimensions we compare the measured E_{0a} with two different theoretical predictions on the finite size behavior of the energy splitting. We find that our numerical data are in favor of the predictions based on the semiclassical dilute instanton gas approximation.

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1 Introduction

In studies of first order phase transitions on finite lattices one faces the phenomenon of tunneling between different states. The tunneling rate is related to the surface tension, which is the free energy per unit area associated with the interface separating these different states. As the surface tension is the fundamental parameter for the nucleation rate in first order phase transitions the determination of it has attracted a lot of attention. Examples are widespread. In d=2, models like the q-state potts model are of interest for statistical physics. In d=3 binary liquids give direct experimental information about the surface tension that can be compared to theoretical calculations using the Ising model as an effective description. In d=4 it is the first order QCD finite temperature phase transition where attempts have been made to extract the surface tension. This list of examples is of course by far not exhausting and many more examples could be found.

Here we study the two and four dimensional Ising models below the critical temperature as examples of a typical system undergoing a first order phase transition between two ordered states. In a cylindrical geometry where the time dimension is much longer than the linear spatial dimension, the Ising system will break into domains along the time direction through tunneling. The inverse of the correlation length along the time direction defines a energy splitting between the ground state and the first excited state. This energy splitting is related to the surface tension [1] which, in turn, is associated with the domain wall energy. The finite volume dependence of the energy splitting has been a long standing problem. A few years ago, a definite finite size behavior for the energy splitting was derived based on a semiclassical dilute instanton gas approximation [2]. The result agreed with an earlier intuitive conjecture by Brézin and Zinn-Justin [3]. Furthermore, a relation between the surface tension and the renormalized parameters was derived in this approximation. This relation was checked in a numerical simulation and good agreement had been found both in four [4] and three dimensions [5].

Recently, Borgs and Imbrie [6] gave a new derivation for the finite size behavior of the energy splitting for a general Ising like system. Their result is claimed to be *exact*. However, it is in disagreement with the instanton calculation.

In this paper we confront both theoretical predictions with a Monte Carlo simulation. We first calculate the energy splitting in the two dimensional Ising model. By comparing to the known exact formula, we demonstrate that the method developed in ref. [4] is very efficient and reliable for calculating the energy splitting. Then we turn our attentions to the four dimensional Ising model.

2 The Ising model

The Ising model in d-dimensions is defined by

$$S = -\kappa \sum_{x \in \Lambda} \sum_{\mu=1}^{d} \Phi_x \left[\Phi_{x+\mu} + \Phi_{x-\mu} \right] \ , \tag{1}$$

where the fields Φ can only assume values ± 1. Here Λ is the volume of the lattice, i.e. TL in d=2 and TL^3 in d=4 with T the time and L the spatial extent of the lattice. Periodic boundary conditions are taken in all directions. The hopping parameter κ is related to the inverse temperature. As is well known, the model eq. (1) can be solved exactly in d=2 [7] and has therefore played the role as a very often used toy model to test ideas and methods. In d=4 the Ising model is in the same universality class as the Φ^4 theory. It exhibits therefore properties like triviality and was used to study at least qualitatively important aspects of the Standard Model physics [8, 9, 4].

The Ising model eq. (1) is symmetric under parity transformation $\Phi \to -\Phi$. For $\kappa > \kappa_c$ with $\kappa_c = \frac{1}{4} \log(1+\sqrt{2}) \approx 0.22036$ in d=2 and $\kappa_c \approx 0.0748$ in d=4, this global Z(2) symmetry is spontaneously broken in infinite volume. We have a double well potential with minima at $+M$ and $-M$. There are two degenerate ground states $|0_+>$ and $|0_->$ which can be intuitively thought of as wavepackets centered around $+M$ and $-M$, respectively. $|0_+>$ and $|0_->$ have no overlap and a complete Hilbert space for the system can be built on either one of these ground states. Assuming we choose $|0_+>$ as the ground state, the system will have a nonzero magnetization $< 0_+|\Phi|0_+ >= M$. If one includes an external source j the magnetization will align with j. With varying external source the system will pass a first oder phase transition at $j = 0$ and the magnetization M jumps from $+M$ to $-M$.

In a finite system the parity symmetry is never spontaneously broken. For $\kappa > \kappa_c$ the $|0_+>$ and $|0_->$ states are no longer the ground states and have finite overlap. A wavepacket centered around one minimum of the effective potential can always tunnel and spread over to the other minimum. The ground state $|0_s>$ is symmetric under parity transformation and may be expressed as

$$|0_s >= \frac{1}{\sqrt{2}}(|0_+ > + |0_- >). \tag{2}$$

The antisymmetric linear combination of $|0_+>$ and $|0_->$ forms the parity odd first excited state $|0_a>$

$$|0_a >= \frac{1}{\sqrt{2}}(|0_+ > - |0_- >). \tag{3}$$

If we set the ground state energy to be zero, there is a small energy splitting E_{0a} between the first excited state $|0_a>$ and the ground state $|0_s>$. This energy splitting is due to the tunneling between $|0_+>$ and $|0_->$ states.

As is well known [1, 10, 11] the energy splitting E_{0a} vanishes exponentially fast with the spatial extent of the lattice and is related to the surface tension σ, $E_{0a} \sim exp(-\sigma L^{d-1})$.

The finite size behavior of E_{0a} can be analyzed by choosing a lattice geometry where the time extent T is much larger than the spatial extent L of the lattice. In this so called cylindrical geometry the system breaks up into domains of different magnetization, separated by interfaces in the spatial direction.

Defining the timeslice operator S_t

$$S_t = \sum_{\tilde{x} \in L^{d-1}} \Phi_{\tilde{x},t} \ , \tag{4}$$

for large enough t the tunneling energy can be obtained from the correlation function

$$< S_0 S_t >= c_1 (e^{-E_{0a} t} + e^{-E_{0a}(T-t)}) \ . \tag{5}$$

We calculated the correlation function $< S_0 S_t >$ numerically in the d=2 and d=4 Ising models in the broken phase. We used the cluster algorithm [12, 13] in its 1-cluster version where we performed 10 updates in between measurements. We used both, the correlation function $< S_0 S_t >$ and its improved estimator version [14]

$$< S_0 S_t >=< \frac{\Lambda}{|c|} \sum_{\tilde{x},\tilde{y}} \Theta(\tilde{x}, t; \tilde{y}, 0) > \ . \tag{6}$$

Here $|c|$ is the size of the cluster C and Θ is the cluster incidence function

$$\Theta(x; y) = \begin{cases} 1 & \text{if both } x, y \in C \\ 0 & \text{else.} \end{cases} \tag{7}$$

To achieve a realistic error for the energies E_{0a} we split the runs into several subruns and fitted the data according to eq. (5) for each subrun. We then determined the values of E_{0a} by the mean and its error of these individual results.

3 The two dimensional Ising model

We have chosen the two dimensional Ising model to test the method of extracting the surface tension from the finite size behavior of E_{0a}. In two dimensions the L-dependence of E_{0a} in the cylindrical geometry is known exactly [10, 7]

$$E_{0a} = \frac{1}{2} \sum_{k=0}^{L-1} \left[\gamma \left(\frac{2k+1}{L} \right) - \gamma \left(\frac{2k}{L} \right) \right] \tag{8}$$

where

$$\gamma(x) = \cosh^{-1} \left[\cosh(2\kappa^*) \cosh(4\kappa) - \cos(\pi x) \right] \tag{9}$$

and κ^* is the dual coupling

$$\tanh(\kappa^*) = e^{-4\kappa} \ . \tag{10}$$

This exact expression has an asymptotic expansion for $L \to \infty$

$$E_{0a} = \sqrt{\frac{2\sinh(\sigma)}{\pi L}} e^{-L\sigma}(1 + O(\frac{1}{L})) \ , \tag{11}$$

where the surface tension σ is given by

$$\sigma = 2(2\kappa - \kappa^*) = 4\kappa - \ln\left[\frac{1+e^{-4\kappa}}{1-e^{-4\kappa}}\right] \ . \tag{12}$$

Our lattices had a geometry LT where $T = 1000$ and L varied from $5 - 16$. We have chosen two κ values in the broken phase of the model, $\kappa = 0.2326$ and $\kappa = 0.2252$. We performed 50,000 measurements with 10 cluster updates in between each measurement. We fitted the spin-spin correlation function eq. (5) and the improved estimator eq. (6) according to eq. (5) and performed a block error analysis as described above. Both operators gave consistent results. We checked that our fit results are stable against varying the start and end point of the fits.

The resulting values of E_{0a} together with the exact formula eq. (8) is displayed in Fig. 1. We find a perfect agreement between the numerical data and the exact formula. This shows that the energy splitting E_{0a} can be extracted from the correlation function very precisely and reliably.

We remark here that although E_{0a} can be measured accurately, extracting the surface tension from E_{0a} is not easy in this case. The surface tension is only clearly defined when L is large enough and E_{0a} can be well approximated by its asymptotic form eq. (11). In $d = 2$ eq. (11) sets in very slowly. For example, at $\kappa = 0.2326$, E_{0a} calculated from eq. (11) is 20% smaller than the exact value even when $L = 16$. In higher dimensions we expect the situation to improve since the asymptotic behavior of E_{0a} should set in much earlier with an error of $O(1/L^{d-1})$.

4 The four dimensional Ising model

It is well known that the Ising model is in the same universality class as the $\lambda\Phi^4$ theory. Using the language of the continuous $\lambda\Phi^4$ field the energy splitting E_{0a} can be calculated in a dilute instanton gas approximation [11]. If we write the bare potential as

$$V(\Phi) = -\frac{m_0^2}{4}\Phi^2 + \frac{g_0}{24}\Phi^4 \ , \tag{13}$$

the energy splitting can be written as

$$E_{0a} = 2e^{-S_c}\left(\frac{S_c}{2\pi}\right)^{1/2}\left|\frac{det' M}{det M_0}\right|^{-1/2} \ , \tag{14}$$

where det' is the determinant without the zero mode and the classical action S_c comes from a single instanton configuration

$$S_c = 2\frac{m_0^3}{g_0}L^{d-1} \ , \tag{15}$$

and the determinants M and M_0 are given by

$$M = -\partial^2 + m_0^2 - \frac{3}{2}m_0^2 cosh^{-2}\left(\frac{m_0}{2}x_4\right) \ , \tag{16}$$

and

$$M_0 = -\partial^2 + m_0^2 \ . \tag{17}$$

In eq. (14) various factors can be understood intuitively. The factor $\exp(-S_c)$ comes from summing over a noninteracting multi-instanton configuration, the $\sqrt{S_c}$ factor comes from an integration over the location of the instantons and the ratio of determinants $det'M/detM_0$ comes from integrating over the Gaussian fluctuations around the classical instanton configuration. The classical instanton action eq. (15) scales with the spatial volume L^{d-1}. The ultraviolet part in the determinant ratio $|det'M/detM_0|^{-1/2}$ will renormalize the bare parameters in S_c and the infrared part was conjectured to contribute an additional factor L^{-1} [3]. Thus the energy splitting has a general form

$$E_{0a} = C_{inst}L^{\omega}e^{-\sigma L^{d-1}} \ , \tag{18}$$

where σ is the surface tension and ω is conjectured to be $(d-3)/2$ under the dilute instanton gas approximation.

Münster has calculated the determinant ratio $det'M/detM_0$ in a finite spatial volume [2]. The result of his work is in agreement with the conjectured form eq. (18) with $\omega = (d-3)/2$. In addition the surface tension and the constant C_{inst} were calculated in terms of the renormalized parameters. For example, in $d = 4$, we have

$$\sigma_{inst} = 2\frac{m_r^3}{g_r}\left[1 - \frac{g_r}{16\pi^2}\left(\frac{1}{8} + \frac{\pi}{4\sqrt{3}}\right) + O(g_r^2)\right] \tag{19}$$

and

$$C_{inst} = 1.65058\sqrt{2\frac{m_r^3}{g_r}} \ . \tag{20}$$

In eqs. (19) and (20) m_r and g_r are the renormalized mass and renormalized quartic coupling respectively. These quantities are input parameters which have to be determined. A high statistic Monte Carlo simulation was performed at $\kappa = 0.076$ [4]. E_{0a}, m_r and g_r were measured independently and the relation given by eq. (19) was confirmed.

Recently, Borgs and Imbrie claimed [6] to have calculated the *exact* finite size behavior of the energy splitting. In $d = 4$ they get

$$E_{0a} = 2e^{-\sigma L^3} \ , \quad \kappa > \kappa_c \ . \tag{21}$$

This formula differs from eq. (18) in two aspects. First, the prefactor in front of $\exp(-\sigma L^3)$ is independent of the volume. Second, the numerical value of the pre-exponential factor equals two and is believed to be independent of κ.

In order to confront both theoretical predictions with numerical simulation results we performed Monte Carlo simulations to determine E_{0a}. In the same manner as in d=2 we studied the correlation function eq. (5) and its improved estimator eq. (6) also in the four dimensional case. Here we have chosen four κ values where the results for $\kappa = 0.076$ are taken from reference [4]. The measured E_{0a} values are listed in Table 1. As mentioned above the values of g_r and m_r are needed as input for the coefficient C_{inst} and the surface tension σ_{inst} in the instanton calculation. For the κ values (beside $\kappa = 0.0760$) used here we measured m_r and λ_r on large lattices in a similar way as in [4]. The resulting values of m_r and g_r can be found in Table 2.

We show the finite size behavior of E_{0a} for all four κ values in Fig. 2. The solid lines are the *predictions* from the instanton calculation eqs. (18), (19) and (20) and the solid circles are our measured E_{0a}. One of the assumptions in the instanton calculation is that the linear size of the spatial volume L is large. Thus we expect the agreement with MC data will only set in when $L > 2\xi$ with $\xi = 1/m_r$ being the correlation length in a hypercubic geometry. This seems to be the case as shown in Fig. 2. Our largest spatial volume is $L = 14$ at $\kappa = 0.0751$ which is not obviously large enough so that the asymptotic behavior for E_{0a} has set in. At $\kappa = 0.0754$ and $L = 12$ we checked that there is 18% finite size effect when T is increased from 120 to 160 and the effect is reduced to 6% at $L = 11$. This means that T should be at least more than 10 times larger than L to suppress the finite size effects in time direction. Thus an increase in L would require a large increase in T which will require a substantial increase in computer time. Given our limited numerical data, it is not possible to determine the power ω of L dependence in the pre-exponential factor in eq. (18). Instead, at each κ value we take 3 data points with the largest L and fit to the form

$$\ln \frac{E_{0a}}{\sqrt{L}} = -\sigma_{fit} L^3 + \ln C_{fit} \ . \tag{22}$$

The fitted results for σ_{fit} and C_{fit} are listed in Table 3, along with χ^2 per degrees of freedom. For comparison we also list in Table 3 the predicted σ_{inst} and C_{inst} values from eqs. (19) and (20). It is clear from Table 3 that the measured σ_{fit} and C_{fit} values are in reasonable agreement with the instanton calculation prediction. Given the fact that the one-loop correction term in eq. (19) contributes from 9% at $\kappa = 0.0751$ to 13% at $\kappa = 0.0764$, it is unlikely that the observed agreement with the fitted numerical results is accidental.

We also tried a fit to the form

$$E_{0a} = C e^{-\sigma L^3} \tag{23}$$

and the results are listed in Table 4. From χ^2 both fits eq. (22) and eq. (23) are of the same quality with a slightly smaller χ^2 for eq. (23). The fitted values for σ are not very far from those listed in Table 3. However, the fitted pre-exponential factor C values are much smaller than 2 and are dependent on the value of κ. This is a contradiction to eq. (21).

A direct comparison to Borgs and Imbrie result is not possible because in eq. (21)

the surface tension σ is not expressed in terms of the renormalized parameters and should be treated as a free parameter. However, since both fits to eq. (22) and eq. (23) give approximately the same values for the surface tension as shown in Tables 3 and 4 and those values are in reasonable agreement with the predicted value σ_{inst} given by eq. (19), we may take σ_{inst} value as an estimate of the true surface tension. If we use the value of σ_{inst} in eq. (21) and setting the coefficient to 2 as predicted by Borgs and Imbrie, the calculated E_{0a} will have a huge difference from MC data as shown in Fig. 3 ($\kappa = 0.0754$).

5 Conclusion

Choosing a cylindrical geometry where the time extent of the lattice is much larger than the spatial extent, we studied the finite size behavior of the energy splitting E_{0a} on periodic lattices. We demonstrated in the two dimensional Ising model that the values of E_{0a} can be extracted from the spin-spin correlation function very precisely. The finite size dependence of E_{0a} was compared to the known exact results. We find perfect agreement between the numerical simulation results and the exact solution for E_{0a} as shown in Fig. 1.

Extending this method to the four dimensional Ising model we confronted our numerical results with two theoretical predictions, one coming from a dilute instanton gas approximation [2], eq.(18) and one recent work, claiming to have obtained the exact finite size behavior for E_{0a} [6], eq.(21). We measured the infinite volume values of m_r and g_r (as they are required as input for the instanton calculation) at four different κ values (see Table 2). The measured values of E_{0a} (see Table 1) agree reasonably with the predictions by eqs. (18), (19) and (20) from the dilute instanton gas approximation as shown in Fig. 2. Our fits to the form of eq. (22) or eq. (23) give comparable χ^2 per degrees of freedom. This suggests that our numerical data are not accurate enough to determine the power of the L dependence in the pre-exponential factor of E_{0a}. However, assuming E_{0a} has the form of eq. (18) with $\omega = (d-3)/2$, the fitted values for σ and C agree well with the predictions given by eqs. (19) and (20) as shown in Table 3. In contrast, a fit to the form eq. (23), shown in Table 4, gives C values that are much smaller than two and κ dependent. This is in contradiction to the result of Borgs and Imbrie, eq. (21).

We conclude that given the choice between the instanton calculation and the result of ref. [6], our numerical data favor the instanton calculation result. Two comments are in order. First our numerical simulations are performed close to κ_c so that the system is inside the scaling region. The instanton calculation is only valid inside the scaling region since the domain walls are treated as continuous surfaces and renormalization language is used. Second, at present we can not determine the value of ω in eq. (18) from our numerical data. Hypothetically, it is possible to have a scenario that E_{0a} takes the form in eq. (23) with a κ dependent C. Close to the critical point, C would be much smaller than two and gradually increases to two when κ becomes large. We emphasize that so far this scenario has no theoretical backing. In order to determine the value of ω further numerical simulation is needed on a larger lattice and with better statistics.

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Table Caption

Table 1: We give the values of the energy splitting E_{0a} as determined from fits to the correlation function eq. (5). The lattice geometry has been TL^3 where $T = 120$ for $\kappa = 0.0760$ and $T = 160$ elsewhere. The values at $\kappa = 0.0760$ (except the L=11 result) are from reference [4].

Table 2: We give the renormalized mass m_r and the renormalized coupling g_r for the four dimensional Ising model for all κ values used. The values for $\kappa = 0.0760$ are taken from reference [4].

Table 3: We take E_{0a} measured on the largest three volumes at each κ value and fit the data according to eq. (22). The fitted σ_{fit} and C_{fit} are listed here along with χ^2 per degrees of freedom. For comparison σ_{inst} and C_{inst} calculated from eqs. (19) and (20) are also listed.

Table 4: Similar to Table 3, but data are fitted to the form of eq. (23). Note C is much smaller than two and dependent on κ.

Figure Caption

Figure 1: The energy splitting E_{0a} in the two dimensional Ising model as obtained from the Monte Carlo simulation. The open symbols are at $\kappa = 0.2326$, the solid symbols are at $\kappa = 0.2252$. The errorbars are smaller than the size of symbols. The lines represent the exact solution eq. (8). Note that no fit is involved.

Figure 2: The energy splitting E_{0a} for the four dimensional Ising model at four κ values. The solid circles indicate the measured E_{0a}. The statistical errors are smaller than the size of symbols. The full curves are the *predictions* from the instanton calculation eq. (18) [2].

Figure 3: The energy splitting E_{0a} for the four dimensional Ising model at $\kappa = 0.0754$. The dashed curve is given by eq. (21) with σ calculated from eq. (19). For comparison the full curve is from the instanton calculation eq. (18).

$\kappa = 0.0751$		$\kappa = 0.0754$		$\kappa = 0.0760$		$\kappa = 0.0764$	
L	E_{0a}	L	E_{0a}	L	E_{0a}	L	E_{0a}
7	0.161(1)	7	0.1345(8)	6	0.1281(4)	5	0.181(2)
8	0.1320(8)	8	0.1015(8)	7	0.0812(3)	6	0.098(2)
9	0.1118(7)	9	0.0761(8)	8	0.04609(2)	7	0.0533(8)
10	0.0944(7)	10	0.0552(9)	9	0.02238(1)	8	0.0223(3)
11	0.0757(8)	11	0.0370(6)	10	0.00902(6)	9	0.00726(4)
12	0.0609(7)	12	0.0270(11)	11	0.0027(3)	10	0.00190(6)
13	0.0509(7)	13					
14	0.0436(15)	14					

Table 1

κ	m_r	g_r
0.0751	0.169(3)	24.0(9)
0.0754	0.264(1)	28.3(6)
0.0760	0.395(1)	30.2(4)
0.0764	0.484(2)	36.3(4)

Table 2

κ	σ_{fit}	σ_{inst}	C_{fit}	C_{inst}	χ^2
0.0751	0.00043(3)	0.00037(2)	0.037(2)	0.033(1)	0.6
0.0754	0.00121(5)	0.00117(3)	0.057(3)	0.0595(7)	3.2
0.0760	0.00358(2)	0.00363(6)	0.101(1)	0.1054(9)	0.4
0.0764	0.00536(6)	0.00543(9)	0.121(5)	0.130(1)	1.6

Table 3

κ	σ fitted	C fitted	χ^2
0.0751	0.00035(3)	0.112(7)	0.4
0.0754	0.00107(5)	0.16(1)	2.7
0.0760	0.00334(2)	0.255(2)	0.1
0.0764	0.00511(6)	0.30(1)	0.9

Table 4